

09/06/2007

Summary of Process for Examination and Modification of the Tier 2 Groundwater Model

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There has been a perception that the length of plumes generated by the Tier 2 groundwater model may significantly over-estimate the length of actual groundwater contamination plumes.

Some of the goals of the investigation included:

Comparison of actual groundwater plume data from Tier 2 sites to Tier 2 groundwater modeling results. This comparison will help determine how the Tier 2 groundwater model has been performing in practice.

If the comparison shows the Tier 2 groundwater model significantly over-estimates actual groundwater plumes, looking at changes to the Tier 2 groundwater model that would produce modeled plumes that are closer to actual results, while still maintaining a factor of safety.

Tier 2 Modeled Versus Actual Plumes

To look at a comparison of modeled versus actual plumes, groundwater data from over 100 Tier 2 sites was examined. The Tier 2 model is a steady state model (predicts the maximum extent of the plume) and for comparison sites with at least 5 years of groundwater sampling data where the actual groundwater plume appeared to have reached its maximum extent were selected for comparison.

For the Tier 2 test sites the modeled or predicted distance downgradient to a chemical target level was compared to the measured distance downgradient to the target level (the measured distance was estimated by contouring actual measured groundwater data).

An example of the results for Benzene are shown below:

Benzene

Target Level (ppb)	# of Tier 2 Sites	Mean Tier 2 Modeled Distance(ft)	Mean Contoured Distance (ft)	Ratio of Modeled to Contoured	% of Contoured > Modeled
5	113	1171	136	8.6	0.0
290	105	273	99	2.8	6.7
1540	94	136	71	1.9	11.7
3080	85	94	53	1.8	14.1
4780	75	74	41	1.8	13.3
9950	45	56	32	1.7	13.3

Using a target level of 5 ppb for Benzene for explanation, the results show that for 113 Tier 2 sites, the average modeled distance downgradient to 5 ppb was 1171 feet, while the actual measured distance based on actual groundwater data (”Mean Contoured Distance”) was 136 feet. The average modeled distance was 8.6 times larger than the average measured distance (”Ratio of Modeled to Contoured”). The column “% of Contoured > Modeled” shows the percentage of the tested sites where the contoured distance to the target level was greater than the measured.

It was noted that the results of comparing the Tier 2 model to measured data depended on the target level. For higher target levels, the “Ratio of Modeled to Contoured” is smaller.

The results were similar for other measures of plume distance. For example, looking at the 95% plume distance (the distance where 95% of the plumes are smaller), the ratio between the measured and modeled plumes were larger than that shown for the average distances above (for the 95% distance for a benzene target level of 5 ppb, the ratio of modeled to contoured plume distance was 11.3 times).

The results for Diesel are:

Diesel

Target Level (ppb)	# of Tier 2 Sites	Mean Tier 2 Modeled Distance(ft)	Mean Contoured Distance (ft)	Ratio of Modeled to Contoured	% of Contoured > Modeled
1200	63	1633	95	17.2	0.0
75000	31	347	50	7.0	0.0
2200000	7	185	52	3.6	0.0
4400000	5	153	54	2.9	0.0
5700000	4	153	60	2.6	0.0
11400000	3	114	57	2.0	0.0

Note that for Diesel the average modeled distance for 1200 ppb is 1633 feet while the average measured distance is 95 feet, with the average model distance being 17.2 times greater than the average measured distance.

The same types of comparison were made for Toluene, Xylenes, and Ethylbenzene. There were not sufficient sites to do a comparison for Waste Oil.

Tier 2 Model Modification

The goal of the Tier 2 model modification was to determine if changes could be made to the Tier 2 model so that modeled results would be more reflective of actual plume sizes, while still maintaining a factor of safety.

The current Tier 2 model is:

$$C(x) = C_s \exp\left(\frac{x}{2\alpha_x} \left[1 - \sqrt{1 + \frac{4\lambda\alpha_x}{u}}\right]\right) \operatorname{erf}\left(\frac{aS_w}{4\sqrt{\alpha_y x}}\right) \operatorname{erf}\left(\frac{S_d}{4\sqrt{\alpha_z x}}\right) \quad (1)$$

The values for first order decay are:

Chemical	λ (1/day)
Benzene	0.0005
Toluene	0.0007
Ethylbenzene	0.00013
Xylenes	0.0005
TEH-Diesel	0.0
TEH-Waste Oil	0.0
Naphthalene	0.00013

Further details on the Tier 2 model can be found in the Appendix B of the Tier 2 guidance.

The proposed Tier 2 model is:

$$C(x) = C_s \exp\left(\frac{x_m}{2\alpha_x} \left[1 - \sqrt{1 + \frac{4\lambda\alpha_x}{u}}\right]\right) \operatorname{erf}\left(\frac{aS_w}{4\sqrt{\alpha_y x_m}}\right) \operatorname{erf}\left(\frac{S_d}{4\sqrt{\alpha_z x_m}}\right) \quad (2)$$

Where $x_m = ax + bx^c$ (3)

Note that the difference in equation (1) and (2) is the use of X_m in equation (2) in place of x in equation (1).

The value of X_m is computed from equation (3), where the values for a , b and c in equation (6) are given in Table 1.

Table 1. Parameter values for equation (3)

Chemical	a	b	c
Benzene	1	0.000000227987	3.929438689
Toluene	1	0.000030701	3.133842393
Ethylbenzene	1	0.0001	2.8
Xylenes	1	0.0	0.0
TEH-Diesel	1	0.000000565	3.625804634
TEH-Waste Oil	1	0.000000565	3.625804634
Naphthalene	1	0	0

The proposed values for first order decay are:

Chemical	λ (1/day)
Benzene	0.000127441
Toluene	0.0000208066
Ethylbenzene	0.0
Xylenes	0.0005
TEH-Diesel	0.0000554955
TEH-Waste Oil	0.0000554955
Naphthalene	0.00013

Note that all other factors remain the same between the current Tier 2 model and the proposed Tier 2 model.

Calibration of the Proposed Model

A number of changes in the Tier 2 model were tested. The parameters for the proposed model (a,b,c, λ) were found by calibrating the proposed model against groundwater data from actual Tier 2 sites. A number of different calibration results were found. The results varied in the ratio of average model to measured distances and the % of contoured distances exceeding simulated distances.

The proposed model results for Benzene are summarized below:

Benzene

Model	Target Level (ppb)	# of Tier 2 Sites	Mean Tier 2 Modeled Distance(ft)	Mean Contoured Distance (ft)	Ratio of Modeled to Contoured	% of Contoured > Modeled
Current	5	113	1171	136	8.6	0.0
New	5	113	359	136	2.6	2.7
Current	290	105	273	99	2.8	6.7
New	290	105	190	99	1.9	8.6
Current	1540	94	136	71	1.9	11.7
New	1540	94	123	71	1.7	7.4
Current	3080	85	94	53	1.8	14.1
New	3080	85	94	53	1.8	7.1
Current	4780	75	74	41	1.8	13.3
New	4780	75	77	41	1.9	5.3
Current	9950	45	56	32	1.7	13.3
New	9950	45	61	32	1.9	6.7

The table shows the results for the Current Model and the New Model for each target level. Note that for a benzene target level of 5 ppb the average contoured distance is 136 feet, the average Tier 2 modeled distance is 1171 feet and the average modeled distance for the proposed model is 359 feet. The ratio of modeled to contoured results has been reduced from 8.6 times to 2.6 times.

It was found during calibration that there was a tradeoff between reducing the average modeled distance and increasing the % of time the contoured distance exceeded the modeled distance. Selecting parameters that decreased the average modeled distance increased the % of test sites where the measured plume size exceeded the modeled plume size. The parameters selected were felt by the software evaluation committee to represent the best tradeoff between the two results.

It should be emphasized that the proposed model still contains a significant factor of safety. For example, for a Benzene target level of 5 ppb the average model distance is still 2.6 times larger than the average measured plume size.

A practical aspect is for a target level of 5 ppb for 2.7% of the 113 test sites the measured plume exceeded the modeled plume size. It should be noted that in practice when this occurs a receptor specific modification is made in the modeled parameters such that the modeled plume meets or equals the measured plume size.

It should be emphasized the results presented are from running the current and proposed Tier 2 model against measured plume data from actual Tier 2 LUST sites.

Appendix A contains the results comparing the current Tier 2 model to the proposed Tier 2 model.

Conclusions

The software investigation committee concluded that the proposed model provides more realistic estimates of plume size, when compared to the current Tier 2 model, while still maintaining a suitable factor of safety.

Appendix A:

Summary results for the current and Proposed Tier 2 groundwater simulation model.

Benzene

Model	Target Level (ppb)	# of Tier 2 Sites	Mean Tier 2 Modeled Distance(ft)	Mean Contoured Distance (ft)	Ratio of Modeled to Contoured	% of Contoured > Modeled
Current	5	113	1171	136	8.6	0.0
New	5	113	359	136	2.6	2.7
Current	290	105	273	99	2.8	6.7
New	290	105	190	99	1.9	8.6
Current	1540	94	136	71	1.9	11.7
New	1540	94	123	71	1.7	7.4
Current	3080	85	94	53	1.8	14.1
New	3080	85	94	53	1.8	7.1
Current	4780	75	74	41	1.8	13.3

New	4780	75	77	41	1.9	5.3
Current	9950	45	56	32	1.7	13.3
New	9950	45	61	32	1.9	6.7

Toluene

Model	Target Level (ppb)	# of Tier 2 Sites	Mean Tier 2 Modeled Distance(ft)	Mean Contoured Distance (ft)	Ratio of Modeled to Contoured	% of Contoured > Modeled
Current	1000	86	196	71	2.8	3.5
New	1000	86	150	71	2.1	2.3
Current	7300	60	81	40	2.0	10.0
New	7300	60	81	40	2.0	3.3
Current	20190	32	48	23	2.1	9.4
New	20190	32	53	23	2.4	0.0
Current	40390	7	44	15	2.9	0.0
New	40390	7	46	15	3.0	0.0
Current	52280	4	42	10	4.1	0.0
New	52280	4	43	10	4.2	0.0

Ethylbenzene

Model	Target Level (ppb)	# of Tier 2 Sites	Mean Tier 2 Modeled Distance(ft)	Mean Contoured Distance (ft)	Ratio of Modeled to Contoured	% of Contoured > Modeled
Current	700	99	141	58	2.4	5.1
New	700	99	115	58	2.0	4.0
Current	3700	42	66	23	2.9	0.0
New	3700	42	61	23	2.7	0.0
Current	46000	2	67	33	2.0	0.0
New	46000	2	63	33	1.9	0.0
Current	91930	1	49	25	2.0	0.0
New	91930	1	50	25	2.0	0.0
Current	118970	1	33	11	3.0	0.0
New	118970	1	34	11	3.1	0.0

Xylenes (no changes in xylenes modeling is proposed)

Model	Target Level (ppb)	# of Tier 2 Sites	Mean Tier 2 Modeled Distance(ft)	Mean Contoured Distance (ft)	Ratio of Modeled to Contoured	% of Contoured > Modeled
Current	10000	58	70	33	2.1	5.2
Current	73000	3	72	33	2.2	0.0

Diesel

Model	Target Level (ppb)	# of Tier 2 Sites	Mean Tier 2 Modeled Distance(ft)	Mean Contoured Distance (ft)	Ratio of Modeled to Contoured	% of Contoured > Modeled
Current	1200	63	1633	95	17.2	0.0
New	1200	63	330	95	3.5	1.6
Current	75000	31	347	50	7.0	0.0
New	75000	31	160	50	3.2	0.0
Current	2200000	7	185	52	3.6	0.0
New	2200000	7	133	52	2.6	0.0
Current	4400000	5	153	54	2.9	0.0
New	4400000	5	121	54	2.3	0.0
Current	5700000	4	153	60	2.6	0.0
New	5700000	4	126	60	2.1	0.0
Current	11400000	3	114	57	2.0	0.0
New	11400000	3	103	57	1.8	0.0

Waste Oil – There were no sufficient Tier 2 site data for Waste Oil. It is proposed to use the same model for Diesel and Waste Oil.